Slides, notes, and exercises at:
https://github.com/cheshyre/nptls-hf

Introduction / Overview of low-energy nuclear physics and nuclear forces

Nuclear Physics Turtle Lecture Series 2025:
Ab initio Hartree-Fock calculations of nuclei

Lecture 1

Matthias Heinz, ORNL

Work supported by:
U.S. DEPARTMENT OF ENERGY
NUCLEI
Nuclear Computational Low-Energy Initiative

About me

Matthias (마티아스)
heinz.matthias.physics@gmail.com

- Travel
- Hiking
- Running
- Climbing
- Food and drinks
- Music
- Video games

About me

Darmstadt

About me

Darmstadt

B.Sc. with Dick Furnstahl

- Nuclear forces
- Similarity renormalization group

About me

B.Sc. with Dick Furnstahl

- Nuclear forces
- Similarity renormalization group

TECHNISCHE UNIVERSITÄT DARMSTADT

M.Sc., Ph.D. with Achim Schwenk

- Nuclear structure
- Many-body methods

About me

B.Sc. with Dick Furnstahl

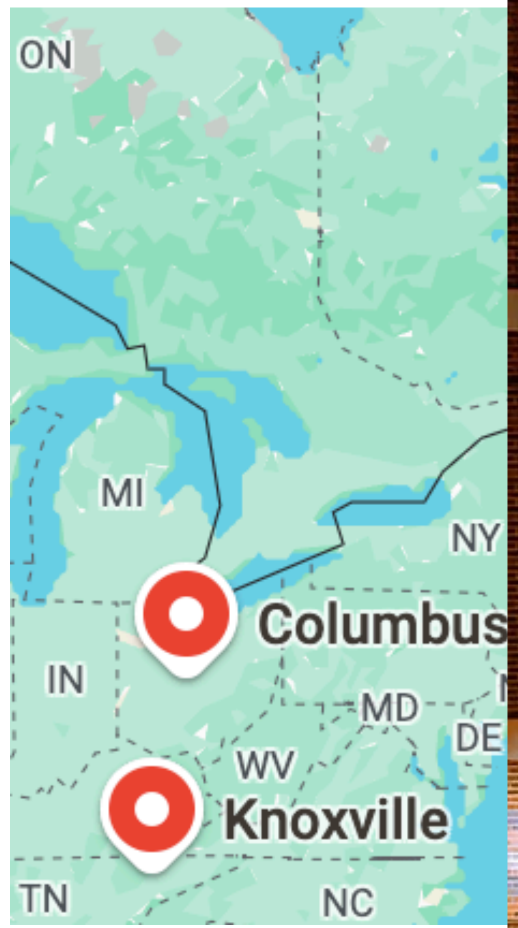
group

Oak Ridge National Laboratory | Leadership Computing Facility

Wigner Fellow at ORNL, Computing & Physics

- **Nuclear structure theory**
- Focus on applications to new physics
- Future interest in nucleosynthesis

About me



B.Sc. with Dick Furnstahl

OAK RIDGE National Laboratory | LEADERSHIP COMPUTING FACILITY

group

Wigner Fellow at ORNL, Computing & Physics venk

- **Nuclear structure theory**
- Focus on applications to new physics
- Future interest in nucleosynthesis

Goals for these lectures

- **Goal: Understand how we can compute nuclei from nuclear forces**
- Hartree-Fock theory is a key ingredient here
- **Priority = Clarity**, please ask questions or slow me down if unclear!

- Programming goal: **Develop Hartree-Fock code for nuclei**
- Ambitious goal: Realistic Hartree-Fock calculations of $^{78}\mathrm{Ni}$

Goals for these lectures

- **Goal: Understand how we can compute nuclei from nuclear forces**
- Hartree-Fock theory is a key ingredient here
- **Priority = Clarity**, please ask questions or slow me down if unclear!

- Programming goal: **Develop Hartree-Fock code for nuclei**
- Ambitious goal: Realistic Hartree-Fock calculations of $^{78}\mathrm{Ni}$

Our approach is same as what is done in current research. No shortcuts!

Overview

Lectures:

- Low-energy nuclear physics
- Many-body theory
- Hartree-Fock method
- Hartree-Fock for nuclei
- Nuclear structure from Hartree-Fock
- Beyond Hartree-Fock

Exercises:

- Hartree-Fock for a schematic Hamiltonian
  - **Goal:** Grow comfortable with many-body problem and formalism
- Hartree-Fock for nuclei
  - **Goal:** Solve HF for nuclei and explore implication for nuclei

Exercise sessions

- **Requirements:** Python3 with numpy, scipy, matplotlib packages installed, run with Jupyter notebook

- **Work in groups, share code, ask questions**
- Reference implementations will be available, and I will provide my solutions after each set of exercises
- All calculations can be done on most laptops (maybe a little patience is required)

Overview of low-energy nuclear physics and nuclear forces

Nuclear Physics Turtle Lecture Series 2025:
Ab initio Hartree-Fock calculations of nuclei

Lecture 1

Matthias Heinz, ORNL

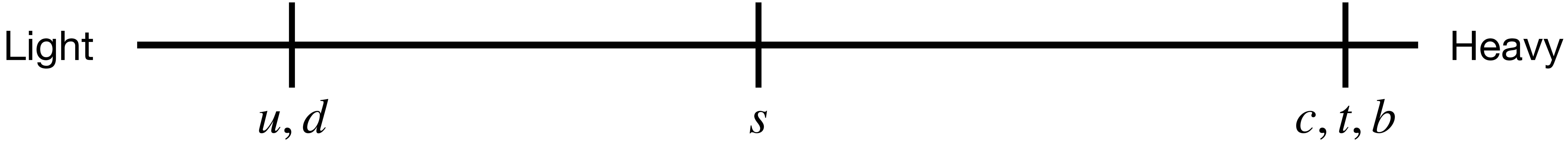
Work supported by:
U.S. DEPARTMENT OF ENERGY
NUCLEI
Nuclear Computational Low-Energy Initiative

Main messages

- Atomic nuclei and nuclear matter are **low-energy systems**
- They can be efficiently described based on **interacting nucleons**
- We can learn about **nuclear forces** from **few-nucleon systems**...
- ... and based on **general symmetry arguments**
- But nuclear forces are **not unique**, but effective descriptions of nature
- **Effective theories** allow us to connect nuclear forces to **QCD**

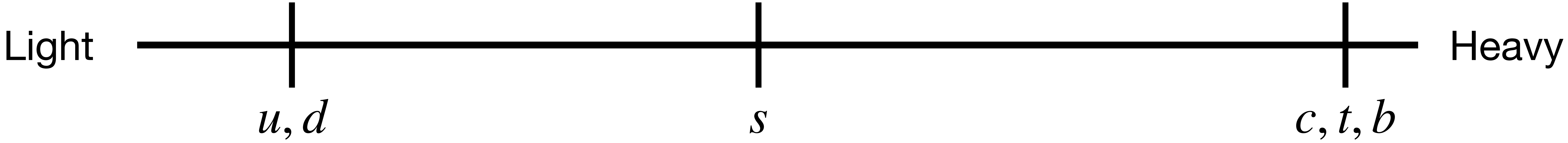
Relevant scales in nuclear physics

Quarks

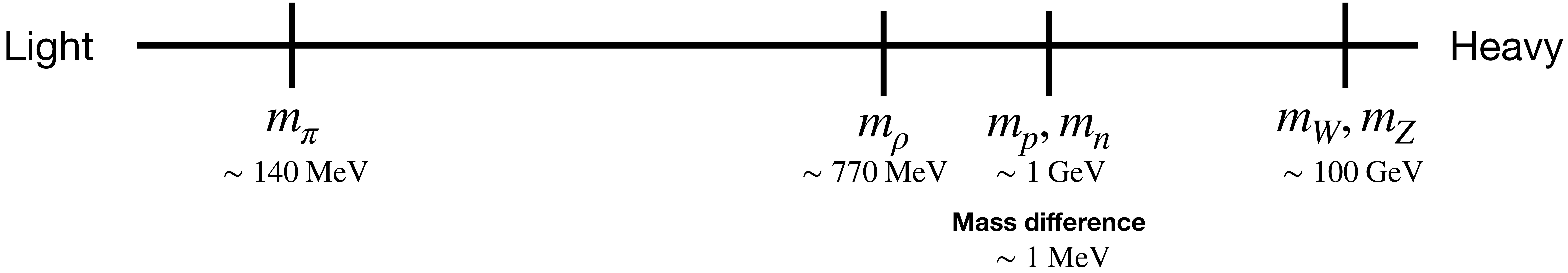


Relevant scales in nuclear physics

Quarks



Hadrons & bosons

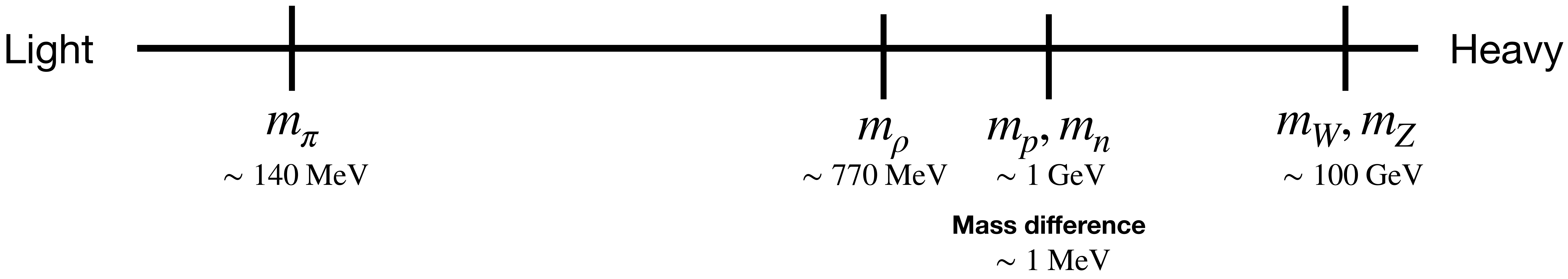


Relevant scales in nuclear physics

What are the relevant interaction energies for nuclei?

How much energy do the nucleons in nuclei have?

Hadrons & bosons



Two-nucleon systems

- Proton-proton:
  - Likely unbound, difficult to measure (Coulomb)
- Neutron-neutron:
  - Unbound
- Proton-neutron:
  - Bound state: Deuteron
  - $E_b = 2.2\,\mathrm{MeV}$ (small!), $R_{\mathrm{ch}} = 2\,\mathrm{fm}$ (large!)
  - Deuteron is **unnatural** system

Two-nucleon systems

- Proton-proton:
  - Likely unbound, difficult to measure (Coulomb)
- Neutron-neutron:
  - Unbound
- Proton-neutron:
  - Bound state: Deuteron
  - $E_b = 2.2\,\mathrm{MeV}$ (small!), $R_\mathrm{ch} = 2\,\mathrm{fm}$ (large!)
  - Deuteron is **unnatural** system

What is natural?

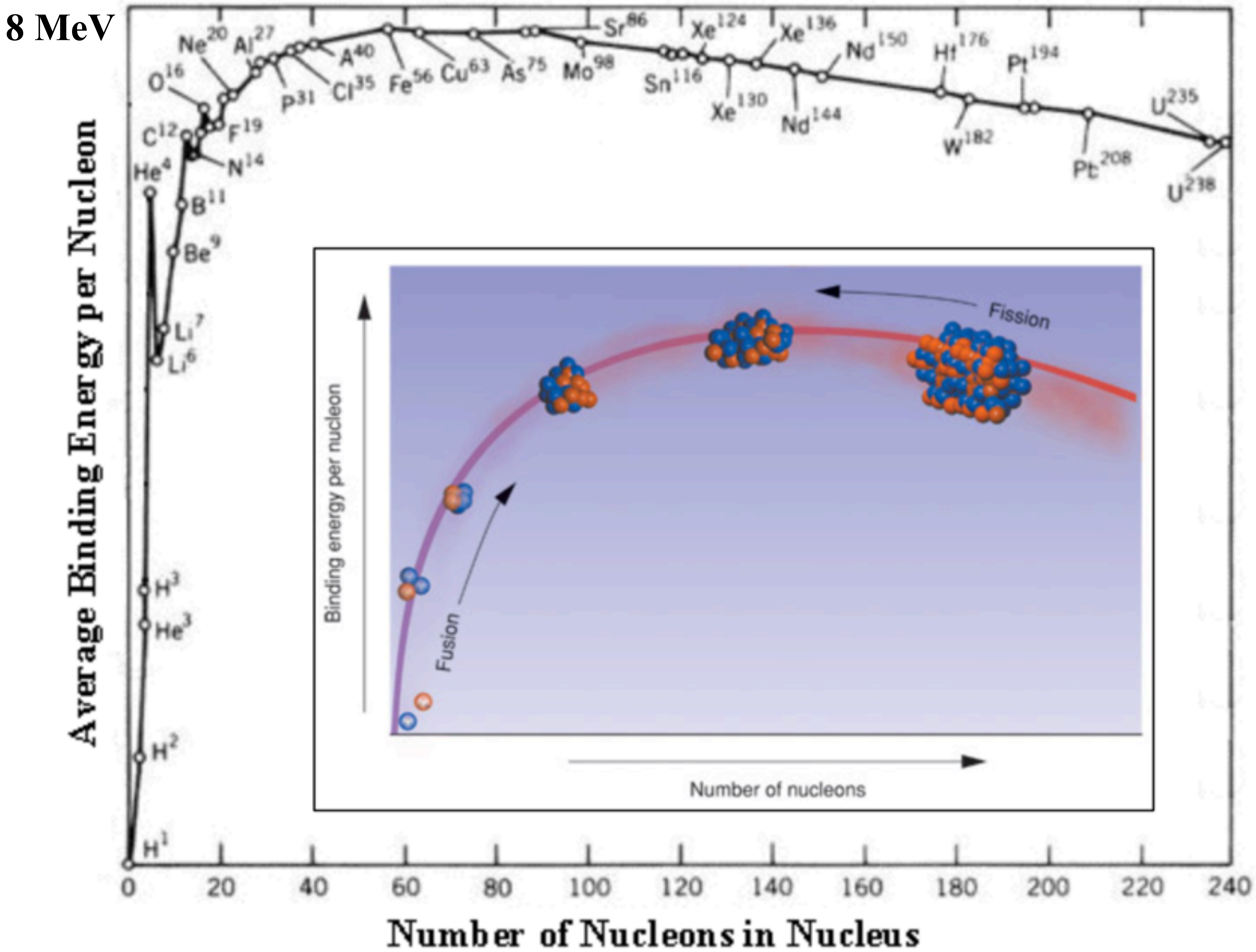
- Estimate from lightest exchange particle: pion

$$E_\mathrm{nat} \sim \frac{p^2}{m_N} \sim \frac{m_\pi^2 c^2}{m_N} = 19\,\mathrm{MeV}$$

$$R_\mathrm{nat} \sim \frac{\hbar c}{m_\pi c^2} = 1.4\,\mathrm{fm}$$

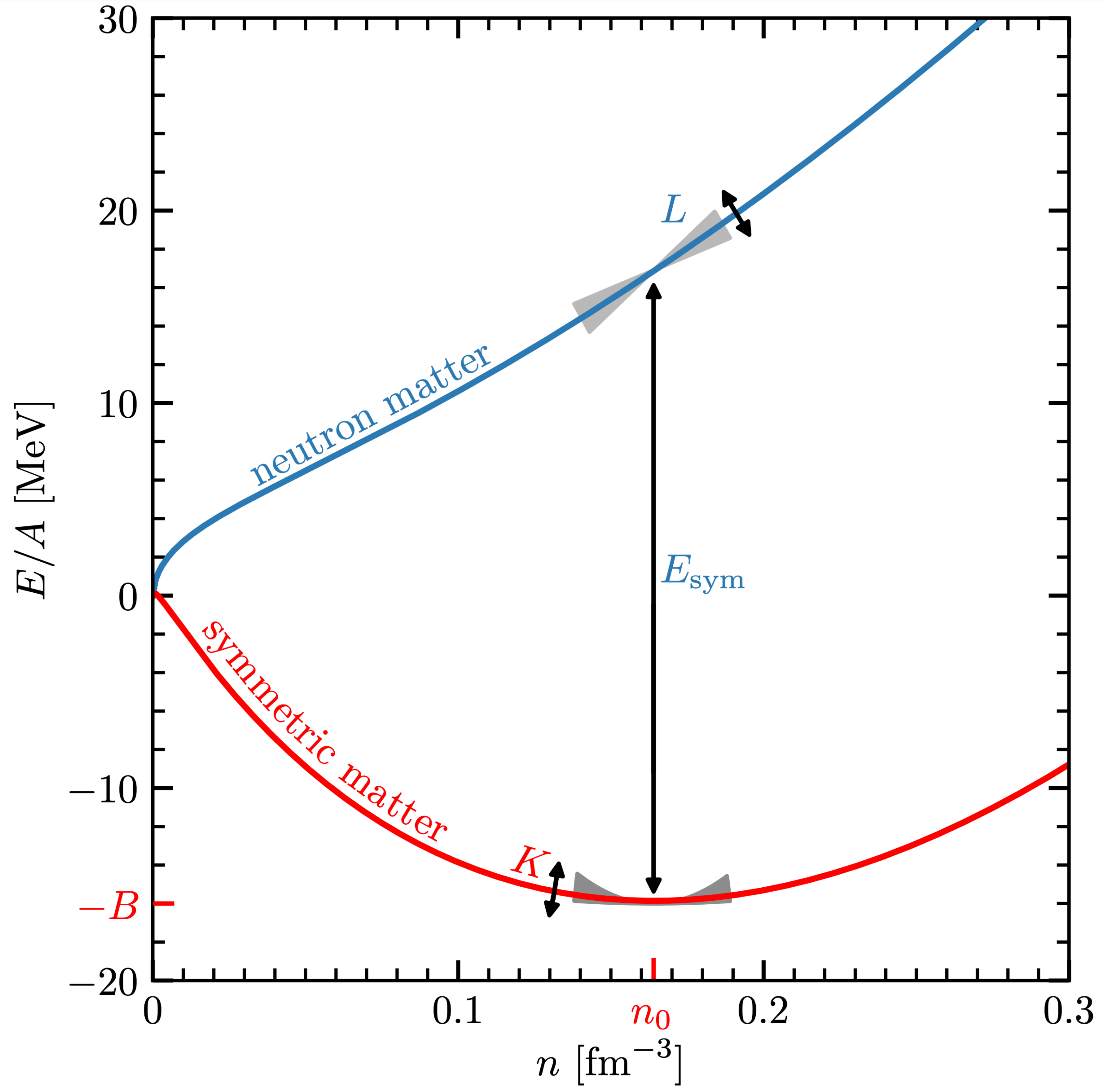
Nuclei

- Nuclei as "liquid drop"
- $E/A \sim 8\,\mathrm{MeV}$
- $R \sim r_0 A^{1/3}$
  with $r_0 \sim 1.3\,\mathrm{fm}$



Nuclear matter

- Theoretical limit of infinite liquid of nucleons
- Symmetric matter ($Z = N$)
  - Saturation at $n_0 \sim 0.16\,\mathrm{fm}^{-3}$
  - $E/A \sim -16\,\mathrm{MeV}$
- Neutron matter (only neutrons)
  - $E/A \sim 16\,\mathrm{MeV}$



Huth, Ph.D. thesis, TU Darmstadt (2023)

The right resolution

- Nuclei and nuclear matter have typical momenta of $\sim m_\pi$
- What about simulations based on quarks?
- **Challenge:** What are the forces between nucleons (and pions)?

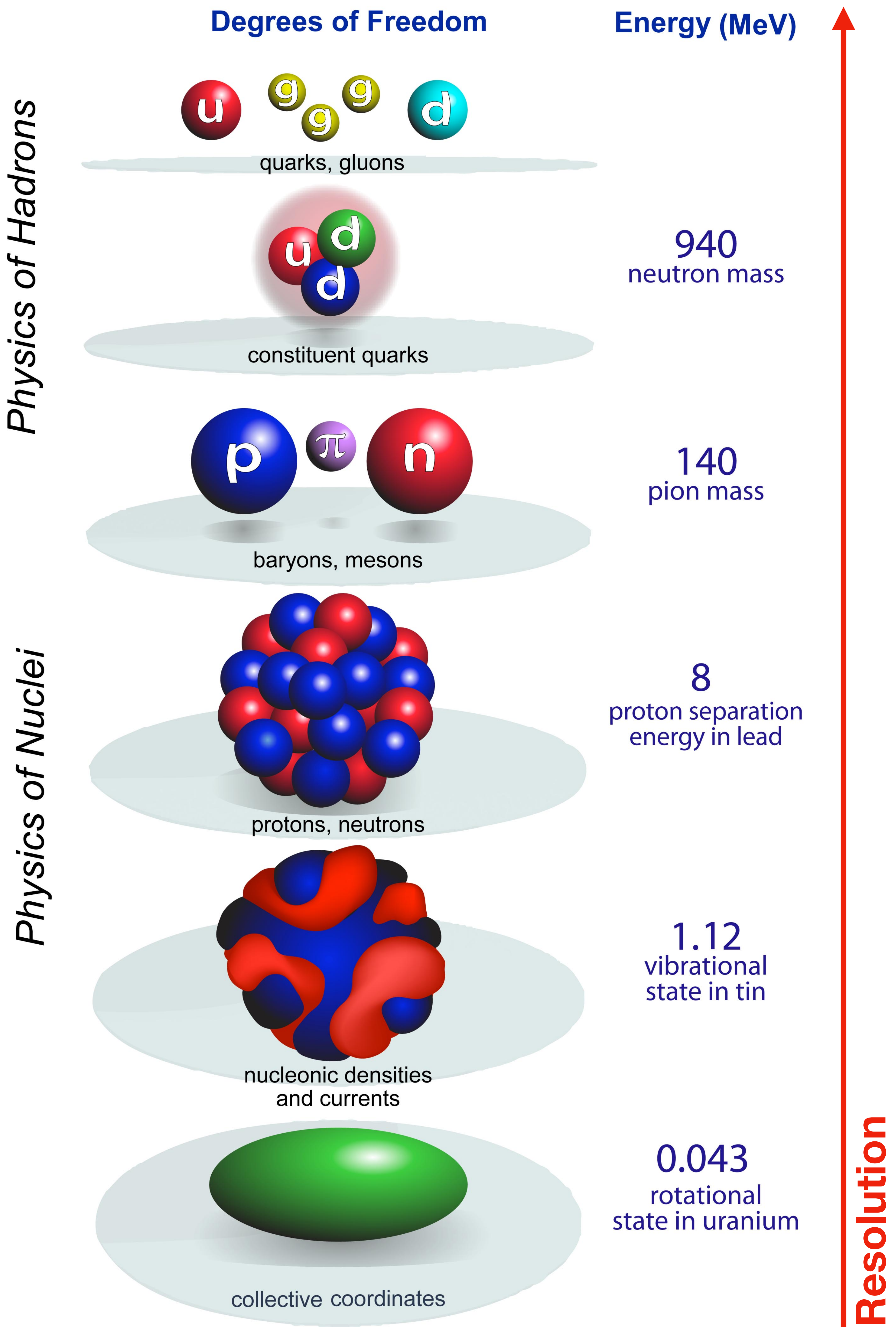


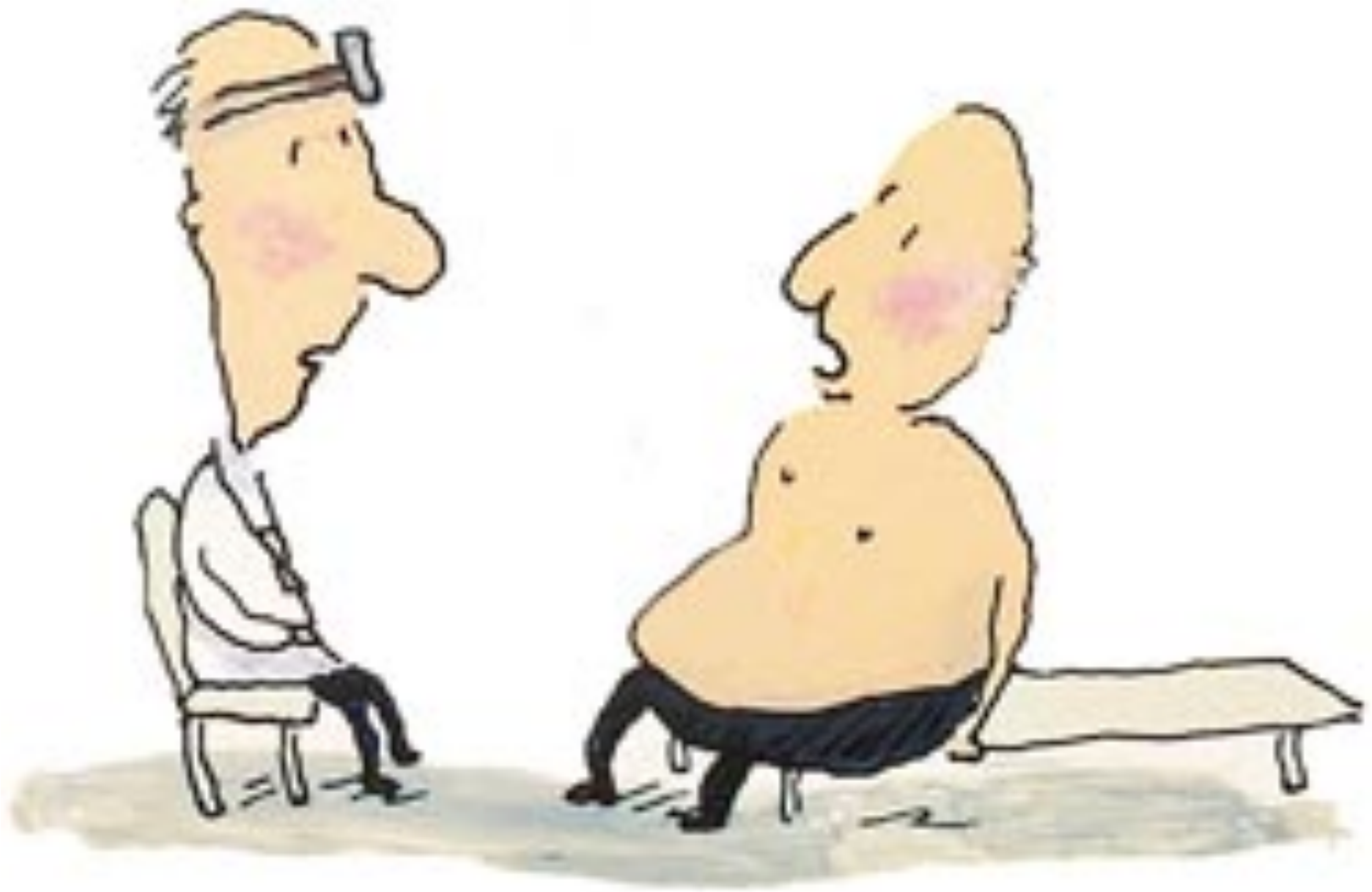
Figure: W. Nazarewicz

Low resolution makes physics easier + efficient

- Weinberg's Third Law of Progress in Theoretical Physics:
  "You may use any degrees of freedom you like to describe a physical system, but if you use the wrong ones, you'll be sorry!"

Low resolution makes physics easier + efficient

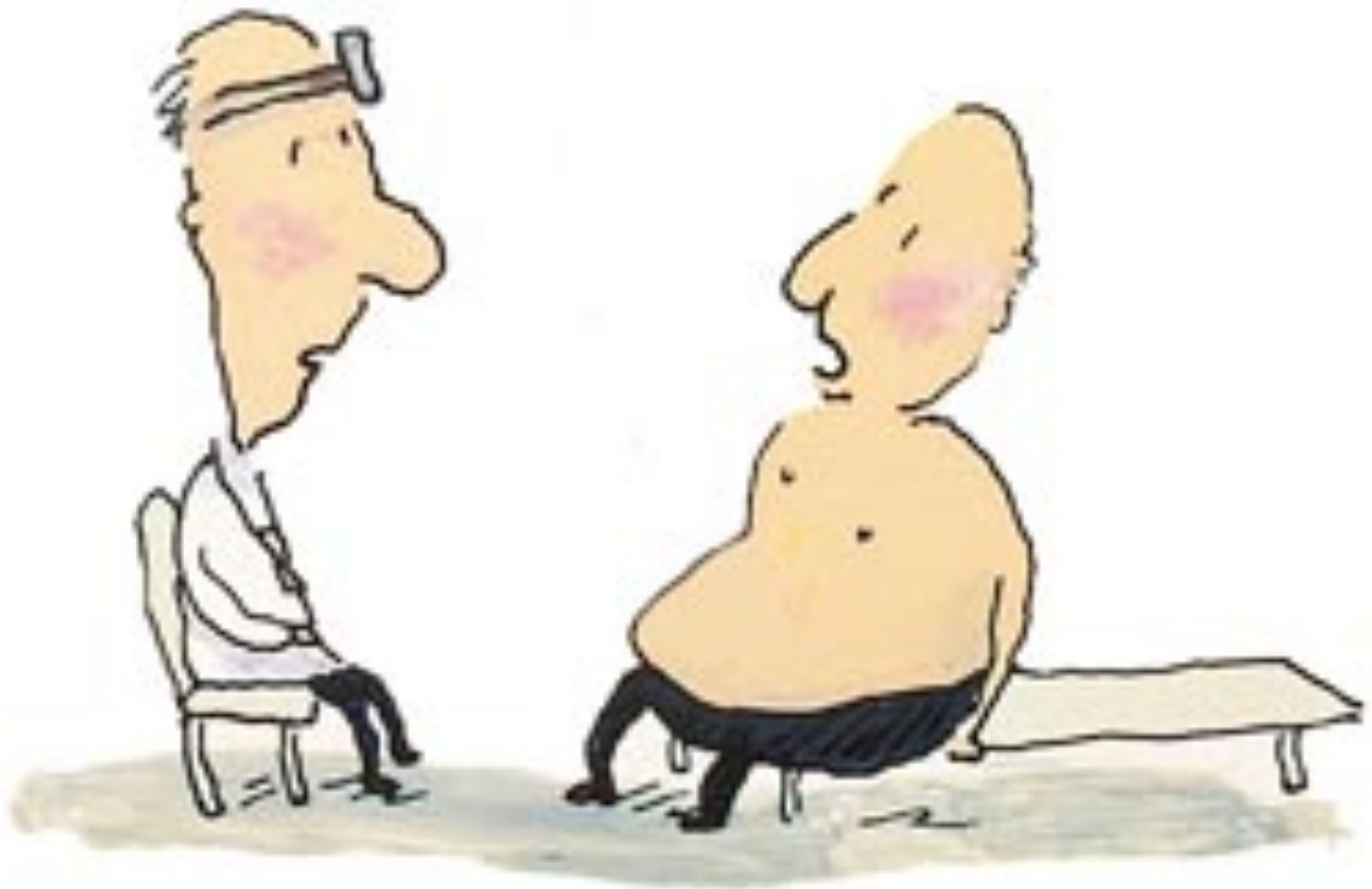
- Weinberg’s Third Law of Progress in Theoretical Physics:
  “You may use any degrees of freedom you like to describe a physical system, but if you use the wrong ones, you’ll be sorry!”
- There’s an old joke about a doctor and patient . . .



Patient: Doctor, doctor, it hurts when I do this!

Low resolution makes physics easier + efficient

- Weinberg's Third Law of Progress in Theoretical Physics:
  "You may use any degrees of freedom you like to describe a physical system, but if you use the wrong ones, you'll be sorry!"
- There's an old joke about a doctor and patient . . .



Patient: Doctor, doctor, it hurts when I do this!
Doctor: Then don't do that.

The right resolution

- Nuclei and nuclear matter have typical momenta of $\sim m_\pi$
- What about simulations based on quarks?
- **Challenge:** What are the forces between nucleons (and pions)?

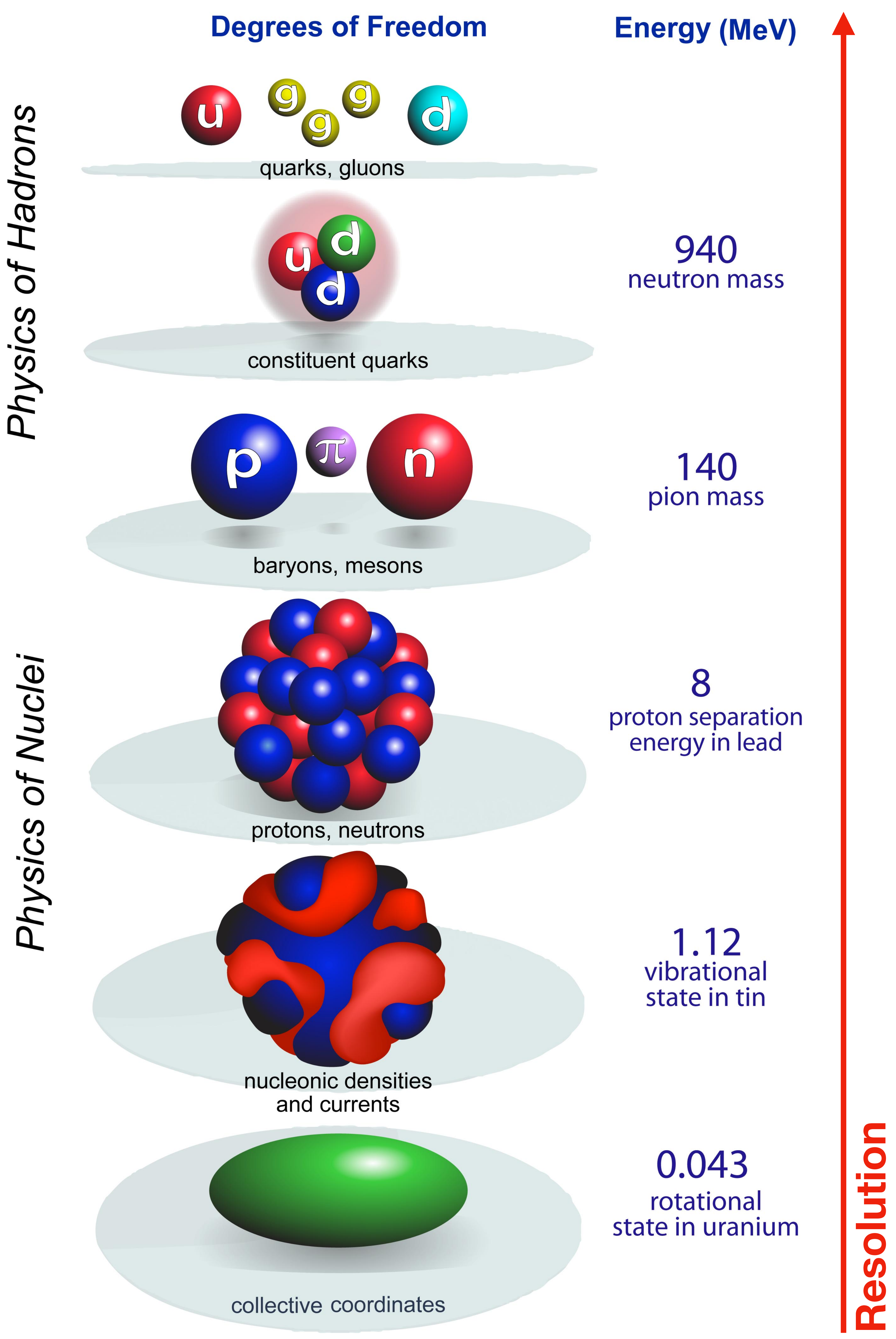


Figure: W. Nazarewicz

Intro to nuclear forces on whiteboard

Summary

- We aim to describe nuclei as **low-energy, strong interaction** systems consisting of **nucleons** as degrees of freedom
- The theory of nuclear forces has rich history with many different approaches
- Modern techniques root **nuclear forces in QCD** through **effective theories**
- Nuclear forces are not unique, many different equivalent versions exist
- For our purposes:
    - **Goal:** From nucleon-nucleon and three-nucleon potentials V_{NN}, V_{3N} solve the Schrödinger equation for nuclei → **Hartree-Fock**